

THE NATIONAL BUREAU OF STANDARDS

Technical News Bulletin

MAY 1973



**Preventing
Flammable
Fabric Accidents**

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Technical News Bulletin

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Cover: In a recent case reported to the NBS Flammable Fabrics Accident Case and Testing System—FFACTS—a young girl climbed up on the stove to reach a bowl of apples. In climbing she turned on the burner, which ignited her pajamas, resulting in serious burns and two months of hospital care. See page 114 for more on FFACTS.

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Technical News Bulletin

THE METRIC CHANGEOVER

NEW NBS DIRECTOR URGES A NATIONAL POLICY FOR METRIC CONVERSION.

On March 19, 1973, Dr. Richard W. Roberts, Director of NBS, presented testimony in support of HR5749, The Metric Conversion Act of 1973. Hearings on this Bill were held by the Science Research and Development Subcommittee of the House of Representatives Committee on Science and Astronautics. Excerpts from Dr. Roberts' testimony follow.

This Bill (HR5749) would establish a national policy of voluntary conversion to the metric system in the United States. It would create the machinery to help guide us through a period of adjustment over the next decade as the use of the metric system in this Nation increases.

Several times in the history of the United States the Congress has wrestled with the question of adopting a national policy to GO METRIC. In 1968, because of growing concern over America's declining position in world trade and the sweeping worldwide adoption of metric units, Congress authorized the Secretary of Commerce to make a study to determine advantages and disadvantages of increased use of the metric system in the United States.

The results of the 3-year study were submitted to the Congress in July of 1971.

- Metric use, already substantial in the United States, is increasing;
- The majority of the manufacturers who participated said that increased metric use would be in the best interests of our Nation; more than 90 percent preferred that this be accomplished through a coordinated national program.

With the Report to the Congress the Secretary of Commerce submitted nine recommendations as follows:



turn page

METRIC *continued*

- That the United States change to the International Metric System deliberately and carefully;
- That this be done through a coordinated national program;
- That the Congress assign responsibility for guiding the change, and for anticipating the kinds of special problems described in the report, to a central coordinating body responsive to all sectors of society;
- That within this framework, detailed plans and timetables be worked out by these sectors;
- That early priority be given to stimulating American schoolchildren and the public at large to think "metric";
- That the Congress foster immediate U.S. participation in international standards activities;
- That to encourage efficiency and minimize overall costs the rule should be that changeover costs "lie where they fall";
- That the Congress, after deciding on a plan for the Nation, establish a 10 year target date by which time the United States shall have become predominantly, though not exclusively, metric;
- That there be a firm government commitment to this goal.

USE OF THE METRIC SYSTEM IN THE UNITED STATES TODAY

It is evident that the rate of increase in the use of the metric system in the United States is greater now than it was when the U.S. Metric Study was made in 1970. Increased metric use is largely in manufacturing, the sector in which the potential exists for the greatest gains in "going metric" and for the greatest losses in not.

Gains are principally of three

kinds. First, a potential increase in exports of manufactured products made to metric standards; predominantly metric countries give preference to metric design products.

Second, there is savings potential when a common design can be used for products made by U.S. companies both here and abroad. If there is to be uniformity of manufacturing procedures it is evident that our inch-pound measurement units must be changed and not the millimeter-kilogram units now so firmly in use worldwide.

Third, changing to metric designs affords the opportunity of greatly reducing excessive varieties and sizes of products. A product with great potential savings is fasteners, used in the assembly of machines and devices of all kinds. But almost every other standard part—spark plugs, electric motors, bearings—has similar potential. Large gains can be realized by redesigning these items optimally in

the light of current engineering practices. Not only can money be saved because of reduced inventories and greater production of each size, but scarce material can be saved.

It is evident that in the 2 years since that report, this Nation has not stood still in relation to the metric system. Major companies like IBM, Caterpillar Tractor, International Harvester, and Honeywell are in the midst of publicly declared metrication programs. General Electric has announced its support of a national metric policy. In mid-February the National Association of Manufacturers' Board of Directors adopted a policy position that "the long-term interests of the United States will be best served by adoption of the International System of Units (SI) and thus be in total harmony with the rest of the industrial and commercial world." The National Association of Manufacturers represents more than 13,000 manufacturers. The U.S.



America has considered going metric since James Monroe. Today, our outmoded measuring system is causing problems in foreign trade, education, compatibility, engineering and other areas.



Chamber of Commerce also recommends adopting a national metric policy.

Nor is the manufacturing community alone in support of metrication. At least 35 major associations—including the National Education Association, the National Grange, the American Association of State Highway Officials, and the American Home Economics Association—have gone on record in favor of going metric. An unofficial analysis of editorial opinion in the lay press last year found more than 90 percent of the nearly 1,000 articles and editorials were pro-metric, with slightly more than 2 percent against. Some 8 percent were merely informative and therefore considered neutral.

The fact is that the United States is already on the road to being metric. Yet we are considerably behind all other industrialized nations.

It is important to recognize that it is primarily industry, not government, that is initiating increased

metric use. The question to be asked is: What is government's role?

The motivation of the Administration in endorsing the Department of Commerce's metric legislation is to make the inevitable changeover as cost effective as possible for everybody—industry, labor, the consumer.

We believe that this can best be accomplished through a national commitment to coordinated voluntary changeover to metric. The Nation should begin as quickly as possible to facilitate U.S. participation in developing the rapidly expanding body of international engineering standards which in effect regulate world trade in high technology products.

In the spontaneous changeover to metric that is already in progress, four basic principles are being followed; care should be exercised to see that they continue to be followed:

(1) The rule of reason. Changes to metric should be made where it is

advantageous to do so; changes should not be made just for the sake of change.

(2) No subsidies.

(3) Voluntary changeover.

(4) Non-governmental initiative.

The major purpose to be served by legislation is to establish a national policy and to create a mechanism for planning and coordinating the changeover on a national scale. For the present, there appears to be no need for the government to take action that encompasses any more than this objective.

The 3-year U.S. Metric Study could not obtain an accurate answer to the question, "How much would it cost the manufacturing industry to convert to the metric system?" Even nations that have made the change have been unable to figure the costs and benefits. Responses from within individual U.S. industries ranged over a factor of 900. The reasons for these wide variations in cost estimates are

turn page

METRIC *continued*

discussed in full in the Manufacturing Industry Interim Report, one of 12 supplementary reports of the study. But, from the study, one conclusion emerged: It will be less costly and the benefits will come sooner if the Nation changes to metric by plan rather than changing sporadically.

MINIMIZING COST AS WE CHANGE TO METRIC

The question of the cost of "going metric" has produced a variety of contentions that are indeed confusing. As pointed out in the U.S. Metric Study,¹ the meaningful comparison of costs is between increased metric use by plan or increased use with no plan. We are steadily increasing metric use and will continue to do so with or without legislation. The meaningful comparison of costs leads to the conclusion that costs and benefits of increasing metric use by plan would be more favorable than those incurred through continued drift into mixed customary and metric usage. What needs to be made clear is that in a planned voluntary program, costs are expected to be less than the benefits that can reasonably be expected to be achieved.

The objective of metric legislation must not be complete conversion to the metric system regardless of cost—instead it must be metrication with minimum cost. We must bear our objective in mind: a predominantly metric country over a decade with changes made only where it is advantageous to do so.

Today we have strong evidence that the cost of changeover to metric is not nearly as great as some people once thought. In addition to experiences gathered from the British changeover now going on, let me cite one example from U.S. industry. John Deere and Company is currently in the midst of a switch to

metric. That company has found that virtually no machine tools have had to be replaced. Conversion charts and/or dual dimensioned drawings can be used to produce items either in customary or metric units. Tool modification—changing scales or mechanical parts—is not as costly as total tool replacement. At the same time, tool replacement is a constant process in manufacturing, and metric tools can be purchased to replace customary unit tools under the normal replacement plan.

A similar situation exists in other areas that would be affected by metrication:

- The automobile mechanic, for instance, has probably already purchased tools that fit metric parts, or will soon do so. The reason, obviously, is that more than 1/4 of the cars on the Nation's highways require metric tools. With a voluntary conversion process over a long period of time, there is no need to scrap customary tools in favor of metric ones.

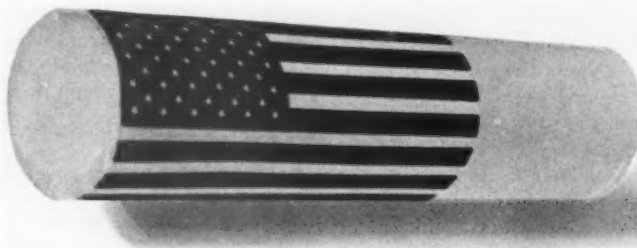
- Metric measuring cups and cookbooks are finding their way into American kitchens these days because foreign culinary arts are well accepted here. Manufacturers of housewares are finding a growing market for metric-labeled or dual-labeled products. More than half of our canned goods are now labeled in both customary and metric units.

- Americans are increasingly exposed to metric language, in everyday commerce and in everyday living. Many of today's products are specified in metric units, like photographic film, prescription drugs, cigarettes, and skis. The Olympic Games are conducted in a base of metric units. We are getting used to buying foreign automobiles on the basis of cubic centimeters displacement. Now, the Cadillac has begun advertising its displacement in metric units in deference to its European competitors.

Not all customary units will necessarily disappear from American language or usage. We can expect, for instance, that horse races will be run in furlongs rather than meters. Under the rule of reason, it may be that land will continue to be sold in acres rather than hectares since real estate is rarely exchanged internationally.

Passage of the Department's Bill (HR5749) providing the machinery to help guide use through the period of adjustment already underway as this Nation changes over to predominant metric use is in the best interest of the United States. I urge that this Congress be the one to articulate the national policy to GO METRIC.

¹A Metric America: A Decision Whose Time Has Come, by Daniel V. DeSimone, National Bureau of Standards Special Publication 345, issued July 1971, 192 pages, \$2.25; SD Catalog No. C13.10 345.





Severe structural damage resulted from the 1971 San Fernando earthquake.

RECOMMENDATIONS TO CUT **DISASTER LOSSES**

Seventy-one recommendations aimed at reducing death and destruction during natural disasters through better building practices have been developed by a national group of experts. The recommendations were developed at a workshop sponsored by NBS and the National Science Foundation.

Property losses in the United States due to natural disasters average more than \$1 billion a year. An even larger part of the problem is human suffering, disruption of production activities, and efforts and expenditures for disaster relief. Though these factors are difficult to quantify, they are among the major losses in any disaster.

The recommendations were

recently released in a report entitled *Building Practices for Disaster Mitigation*¹ by the Center for Building Technology. The suggestions are directed at policy makers, standards writers, and the building industry. Experts at the workshop included engineers, physical scientists, architects, planners, social scientists, economists, and public administrators from all over the country.

The recommendations call for improved building codes to assure public safety during natural disasters, better planning, and additional research.

One recommendation urges restructuring federal disaster assistance to provide incentives for

minimizing disaster damage through improved building practices and reducing present incentives when risks are ignored.

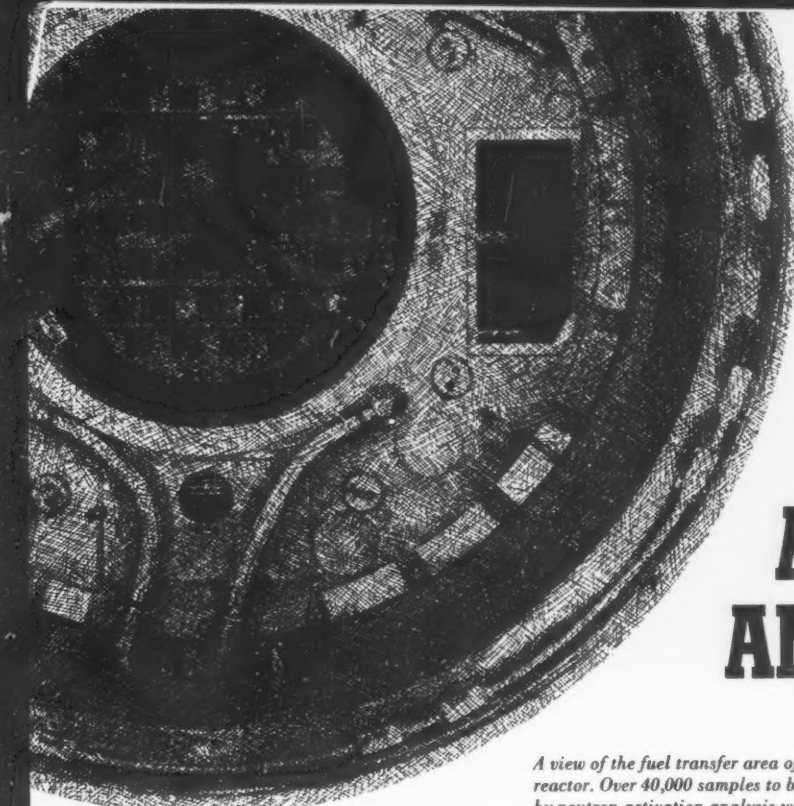
Another recommendation suggests that codes, standards, and contracts should recognize the degree of risk inherent from natural disasters and specify the degree of protection offered by the specific structure.

Earthquakes, extreme winds, and other dynamic hazards are covered in the 475-page report. The study is part of a major cooperative effort aimed at closing the gap between building research and practice. The program involves federal agencies like NBS, NSF, and the Defense Civil Preparedness Agency, as well as professional organizations, the academic community, state and local governments.

As part of the National Bureau of Standards' continuing program, the Center for Building Technology has long been conducting on-the-scene investigations into the performance of buildings under a variety of conditions, including hurricanes, floods, tornados, and earthquakes.

The government's interest is significant because more than a third of all U.S. building construction is federally financed—directly or indirectly. Besides this investment, the government has statutory responsibilities like those set forth under the Federal Disaster Assistance Program. The magnitude of this commitment can be seen in the 1971 San Fernando earthquake where the government-funded nonrepayable reconstruction loans totalled nearly \$200 million.

¹ NBS Building Science Series No. 46, *Building Practices for Disaster Mitigation*, is now available through the Superintendent of Documents, Government Printing Office, Washington, D.C. 20401, for \$5.30.



THE ULTIMATE CONTRIBUTION OF NUCLEAR ACTIVATION ANALYSIS*

A view of the fuel transfer area of the NBS reactor. Over 40,000 samples to be analyzed by neutron activation analysis were irradiated in the reactor in 1972.

What is the real impact of Activation Analysis on analytical chemistry today? In other words, what are the unique characteristics of this method that make it important to present-day analytical chemistry? Where do our efforts fit into the broad spectrum of scientific competences in analytical chemistry?

ANALYSIS—OUR OBJECTIVE

We must remember that we are talking about *Activation ANALYSIS*. This is much different from nuclear activation in general, or radiation detector studies, or computer resolution of spectra, or indeed, radiochemical separations, *per se*. The ultimate goal of ANALYSIS (indeed the only true purpose) is to provide measurement values on real samples of significance.

*Excerpted from a speech given by Dr. W. Wayne Meinke, Chief of the Bureau's Analytical Chemistry Division, at the 4th International Conference on Modern Trends in Activation Analysis held in Saclay, France, October 1-6, 1972. Proceedings to be published.

In 1933, one of my predecessors at the Bureau, Dr. G. E. F. Lundell, wrote a very interesting article entitled, "The Chemical Analysis of Things as They Are." He said he used the title because so many articles on analytical subjects deal with "The Chemical Analysis of Things as They Are Not." In this article he drew the distinction between analysts and determinators—and he sketched a future life where heaven for the determinators would contain a shelf on which there was one reagent infallibly specific for each element.

Today the field of analytical chemistry is much more complex and the analytical chemist is called upon to give much more information on a sample than was required in 1933. However, as I look at the field of analysis, I still see many "determinators" who are all too willing to put their faith in an esoteric and expensive piece of measuring equipment, preferably controlled by a

computer, which spews forth results at a tremendous rate, and often even plots the graphs and tables for final publication without the benefit of human hands.

Today the general public has been mesmerized into thinking that if it's big, expensive, automatic, and fast, it must be good! Ignore the questions of calibration, of standardization, of accuracy. The machine must be right! Unfortunately, I find many times that well-informed scientists are almost as gullible. It is very distressing to find research scientists and analysts who have persuaded themselves that such is the case in their own experimental field.

I maintain that it is absolutely essential for anyone engaged in analytical chemistry to keep in mind the ultimate end product of his work—i.e., *a meaningful analytical measurement on a real, practical sample.*

Today many decisions that will

eventually determine the quality of life in this world of ours must be based on analytical results. Governments establish legal limits for ambient pollutants in the atmosphere; they legislate maximum operating levels for emissions from automobiles and power plants; they show great concern about levels of pollutants in the waterways; and they are beset from all sides to establish limits to organic and inorganic contaminants in consumable materials ranging from foods to gasoline, from tuna fish to coal.

Only by providing accurate analytical data can we begin to work out of the morass of confusion. Unfortunately, today we find inaccurate analytical data being used as the basis for even less reliable pharmacological data, which in turn is used in the development of an overall model of a pollutant system. Often, then, environmentalists and members of the "establishment" use the same "scientific" data to support completely opposite hypotheses. The net result is that the public loses confidence in science and technology because it appears to furnish no absolute answers.

The time is past when order of

magnitude numbers are important or are even of interest for analysis. Whether we like it or not, most of the hard decisions that need to be made in the pollution field require analyses with errors far below 50 percent, often as low as a few percent. I am convinced that *accuracy* in high-sensitivity analyses must be improved by factors of two or 10 or even more if we are to meet the demands upon us. At the very least I believe that the end result of the work of every analytical chemist should be a number with a plus or minus accuracy error limit assigned.

ACCURACY THROUGH STANDARD REFERENCE MATERIALS

The ultimate goal of analytical measurement is a numerical result of known accuracy. Precision studies can be interesting, but in the real world, accuracy is the truly important criterion. Thus it is incumbent upon analytical chemists to study in detail the biases of their methods and procedures.

An excellent means of studying the biases—and thus the accuracy—of a given analytical method is through the use of Standard Reference Materials (SRM's). At

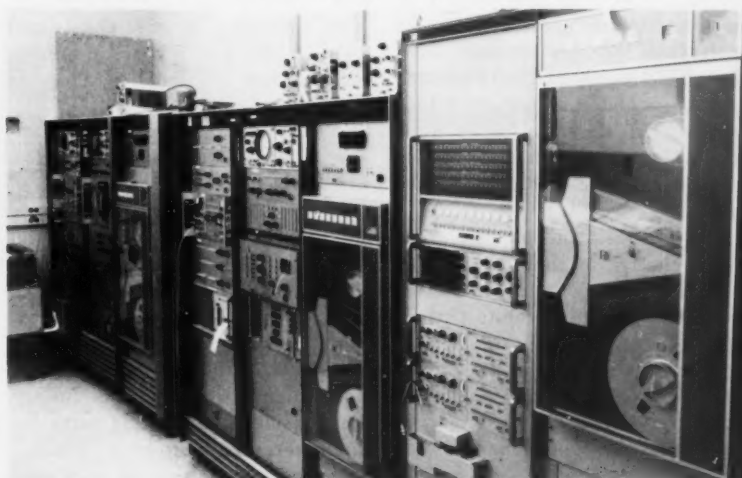
NBS we have a long history of providing, in quantity, such certified materials of guaranteed homogeneity to calibrate a measurement system.

The first NBS standard samples were steel chips issued in 1906 to standardize wet chemical analyses. More recently many NBS SRM's have been developed to calibrate instruments such as pH meters, x-ray and emission spectrographs, etc. In the field of trace analysis we have now developed several certified SRM's which can be used by the trace analyst to calibrate his methods and to study the biases in his particular analytical system.

Certification of a value for an SRM guarantees the accuracy of that value. This is inherent in the certification process wherein a certified number must be the result either of two independent analytical measurements or of measurements by two completely independent laboratories using a referee-type method for which overall errors and biases have been established.

By concentrating his effort on studies of a few good SRM's of proven homogeneity the trace analyst will be able to upgrade his understanding of the biases of his

William Kinard processes data on a minicomputer. The data are taken and recorded by the pulse height analyzers on the left.





Most biological samples are freeze dried prior to neutron irradiation to reduce the evolution of gaseous decomposition products.

methods and hence the accuracy of his methods.

THE PRESENT STATE OF TRACE ANALYSIS

This brings us then to a discussion of the present state of trace analysis. The literature abounds in reports of ultra-trace analyses at the ppb level or lower, with special new instrumentation and techniques and/or adaptations of older methods. Unfortunately, many of these articles are not describing the analysis of "things as they are." They describe theoretical sensitivities, extrapolated values, or values for distilled water or other ideal systems, rather than measurements in the real world of practical samples.

The scientific and popular press are no better in that they report analytical values with no error limits and impute absolute perfection to the number reported. Statements in newspapers in the United States that certain tuna fish were found to contain 0.76 ppm of mercury made no mention of the fact that such mercury analyses are so dif-

ficult that they could easily be in error by as much as 50 percent. The major discussions on DDT contamination in our country a few years back failed to indicate that DDT analyses in water pollution studies can often be in error by considerably more than 50 percent.

Since there are no International Critical Tables to which one can refer to determine the status of analysis in the trace area, one is forced to make one's own estimates. The following is my considered opinion based on 9 years of immersion in the problems of accurate measurements at NBS.

I believe that, on most real samples, trace element analysis below the ppm level gives values of questionable accuracy. All trace methods of analysis except for activation analysis must deal realistically and directly with problems of blank contamination. Past experience has proven that to simply make corrections for blanks does not suffice in trace analysis. Indeed we consider the limiting error for any determination to be \pm "Blank." For accurate analysis we must take

particular care to minimize the sources of contamination.

Contamination comes from three different sources: the surroundings, i.e., the room and the individual scientist himself; the reagents; and the containers used in the analysis.

Admittedly, there may be certain practical trace analyses where only minimal handling is required and where the measurement technique has such high discrimination that good results can come directly out of the measurement. However, in general I am rather cynical about glowing reports on ultra-trace methods. My experience has told me to hold suspect any numbers below the ppm level resulting from any method (except activation analysis) where the analyst has not taken precautions to work in special clean environments with special clean suits, ultra-pure reagents, and special purity containers.

PRESENT STATE OF ACTIVATION ANALYSIS

Now let us take a similar look at activation analysis. First let me draw a distinction which I feel must be made. I believe that *the term activation analysis should be confined to the description of procedures which involve not only nuclear activation and measurement with a detector but also radiochemical separations.* For procedures that involve only nuclear activation and detector measurements I would use the term *Activation Spectrometry* because it is completely analogous in principle to optical-emission spectrometry, infra-red spectrometry, Raman spectrometry, etc.

Activation spectrometry has the advantages as well as the disadvantages of other types of spectrometry that have been with us for many years. It is rapid, it is clean (no chemical reagents are required), it can be readily automated, and it can be developed into a reasonable survey method to give analytical values for a number of elements at

the same time. On the other hand, it has the same disadvantage as these other spectrometries. At certain levels of trace concentration the background of unwanted contaminants overwhelms or distorts the signal from the desired constituent and it becomes difficult or impossible to give accurate analytical values without large numbers of certified standard matrices.

Now let us look at the situation in activation spectrometry. A number of different excitation sources available will excite components of a sample to different levels, in a fashion quite similar to the different types of emission flames, plasmas, sparks, arcs, etc. Once activated the sample is measured with a discriminating detector. Fortunately in activation spectrometry there is a delay time between activation and measurement that gives additional flexibility, but the limiting factor remains the discrimination with respect to neighboring species that can be obtained with the detector system. And no large reservoir of certified Standard Reference Materials is available to assist in calibrations.

It is my observation that no matter how theoretically possible it is to extend the sensitivity of activation spectrometry to the ppb level or beyond, in most practical samples there remains a "credibility" cutoff

Working in a laminar flow clean hood to prevent contamination, Donald Becker prepares a sample for irradiation.



between 1 ppm and 0.1 ppm. This is quite similar to the cutoffs we see in other types of spectrometry. To go below this it is necessary to do chemical separation in exactly the same way that one needs to do chemical preparation of preconcentrations to extend other spectrometries below the ppm cutoff limit.

Activation analysis, i.e., nuclear activation combined with radiochemical separation and discrimination with a good detector, could lead the way to accurate measurements at high sensitivities. Properly performed, activation analysis can reduce or almost eliminate many blank problems, and therefore should be the target method for analyses at the 10 ppb level and below.

In practice, however, we see that a large fraction of the measurements in this field are made by activation spectrometry with an accuracy cutoff around the ppm level. For many of the remaining measurements, unfortunately, the chemistry is not yet well enough under control to meet the ± 10 percent precision limit. *Nevertheless, I firmly believe that the true challenge for activation analysis in the next decade is the extension of accurate trace analytical values to the ppb levels.*

There is a crying need throughout the world for baseline measurements of inorganic contaminants in a wide variety of materials ranging from seawater to blood and from foods to air particulates. To meet this need the activation analyst must not only capitalize on his lack of blank corrections after irradiation but must pay particular attention to the handling of the sample before irradiation. Activation analysis is able to provide the most power toward high-sensitivity analysis when there is a bare minimum of preliminary handling between sampling and irradiation.

In the long run this is the princi-

ple advantage of activation analysis. Today other methods have almost the same calculated sensitivities and surely about equal practical sensitivities, yet no others, I believe, permit unlimited handling without fear of contamination after excitation and before the final detector measurement.

It is true that many reactors today will not accept samples unless they are specially dried or prepared in a certain way. However, if as much effort had gone into the design of irradiation facilities and techniques during the last decade as has gone into detector discrimination and computer programming of the output of detectors, there would be no problem today in handling special types of irradiations. Creative engineering is all that is required, and I believe this is a place for advancement in the future!

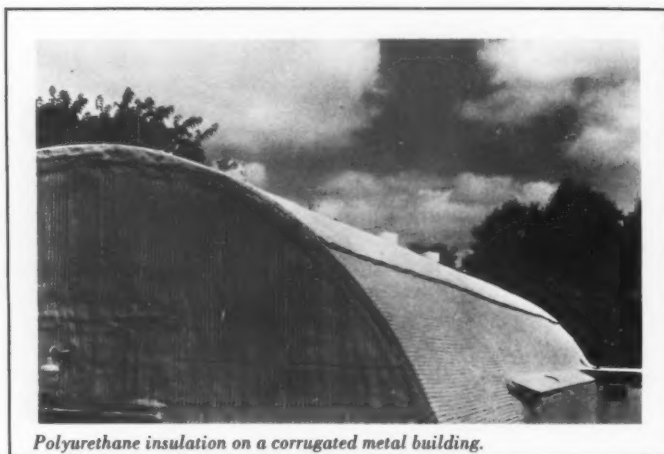
Some concern must be shown in activation analysis for competing reactions, shielding of neighboring nuclei, etc., as well as for reproducibility of counting geometry. These factors, minor at error levels of 10 to 25 percent, become more important when the accuracy limits are extended to 1 percent. However, it would appear that the major strides in extending the meaningful sensitivity for activation analysis will come through improvements in manipulations between the time of sampling and the end of irradiation.

CHALLENGE FOR THE FUTURE

Resolve to make your efforts applicable to the analysis of "things as they are" and avoid unfounded extrapolations, assertions based on ideal systems, etc.

Together we must strive to push to higher and higher sensitivities the limits of accurately known measurements. The results are not only of academic interest! Indeed they are urgently needed to help provide the foundation for a reasonable system of understanding of our environment.

Foam Polyurethane Roofing Systems



Polyurethane insulation on a corrugated metal building.

New guidelines for selection and use of foamed-in-place polyurethane roofing systems have been published by the Bureau.

The use of this type of roofing in the United States is increasing at a rapid rate, but in spite of its wide use, little unbiased information has been available to guide builders and consumers in specifying, selecting, applying, and evaluating the performance of these innovative roofing systems. The new "Guidelines for Selection of and Use of Foam Polyurethane Roofing Systems"¹ were developed by William C. Cullen and Dr. Walter J. Rossiter, Jr. of the Center for Building Technology. They surveyed the state of the art of

polyurethane roofing technology in a study sponsored by the Naval Facilities Engineering Command, U.S. Navy; the Directorate of Civil Engineering, U.S. Air Force; and the Office of the Chief of Engineers, U.S. Army.

Almost a hundred roofs in actual use were inspected in many areas of the United States—from the relatively mild climate of California to that of northern Alaska. The inspected roofs ranged from horizontal to vertical and varied in size from a few squares* to more than 3 acres (130,680 square feet) in area. Several varieties of substrates used

in the urethane systems, including weathered built-up roofing, were examined. Leading roofing contractors, including spray foam applicators, were interviewed to learn their experiences and opinions on the application and performance of urethane roofing systems. Opinions of owners and users were also solicited. Private and public sectors became involved as opinion givers ranged from housewives to plant engineers responsible for urethane roofing systems several acres in area. Data concerning the effect of hailstones on polyurethane roofing systems were supplied from previous experiments at NBS in which simulated hailstones were shot by a

*One square of roofing is equal to 100 square feet.

compressed air gun onto various test samples of urethane roofing material.

To compliment information developed from in-service data sources, a member of the investigating team completed a comprehensive literature survey concerning polyurethane foams.

RESULTS OF STUDY

NBS investigators found that even though they confined their study to rigid (rather than flexible and resilient) polyurethane foams, they encountered a very large variety of foams and many variations in how they are formulated. Moreover, they discovered that changing the proportions of reactants (without changing the reactants themselves) can affect the resultant foam and its properties. They found it difficult to generalize about the properties of rigid foam, so the properties of rigid polyurethane foams are presented in synopsis form in the Guidelines. Each property has been covered in considerably more detail in the literature.

Among the properties important to roofing applications are compressive strength, thermal and photolytic stability, insulation, flammability, impact resistance, and weathering. These properties are summarized below:

● **Compressive Strength.** This property depends on both the density of the foam and the shape of the gas cells within it. Density is the more important factor. As density increases, foam strength increases. In most applications foam density ranges from 1.5 to 2.5 pounds per cubic foot. At 2.5 to 3 pounds per cubic foot compressive strength is 40 to 50 pounds per square inch. The compressive strength of rigid foams decreases with increasing temperature until they become soft and flexible when surrounding temperatures reach 130 to 150 °C.

Above 150 °C most rigid foams have no load bearing capacity but can still possibly support their own weight.

● **Thermal Stability.** As organic polymers, polyurethane foams are susceptible to thermal degradation. But those found in the study can maintain stability at temperatures much higher than those usually encountered on roofs. No information could be obtained regarding heat aging and long-term temperature stability at temperatures normally found on roofs.

● **Photolytic Stability.** Although little published literature exists on this subject, it is well known rigid polyurethane foams of the type used for roofing generally yellow and deteriorate during exposure to sunlight. For roofing use, these foams must be protected by covering them with another material or by painting their exposed surface.

● **Insulation.** The low thermal conductivity (K-factor) of polyurethane foam is one of its most important properties. In fact, a good insulating foam's K-factor is at least twice as low as the best of other insulations. However, the initial K-factor increases somewhat with time and it varies depending upon aging conditions.

● **Flammability.** Rigid polyurethane foams are combustible but the degree of flammability can be altered by physical and chemical flame retardants. Variations in foam formulation can also alter flame retardancy. Before using a foam its flammability must be evaluated.

● **Impact Resistance.** High impact resistance is important, since it prevents roof damage from falling objects such as hail, tools, tree limbs, and the like. Review of the literature revealed little on this subject, but NBS experiments with the compressed air gun indicated that, aside from the foam formulation method used, density of substrate and rigidity of underlying support

had a direct bearing on impact resistance.

● **Weathering.** This is one area in which data is completely lacking in the literature. Although it is a recognized fact that rigid polyurethane foam sprayed on a roof must be protected from ultraviolet radiation (a component of sunlight) by covering or coating, articles describing this could not be found. Also, no information was available comparing the outdoor behavior of foams covered with various materials.

PERFORMANCE SPECIFICATIONS

The complexity of rigid urethane foams and coating systems and the lack of data about performance, durability and long-term weatherability were major constraints in developing adequate material specifications for urethane foams and protective coatings.

The NBS investigators developed a "performance approach" to define acceptable service, rather than set limiting values for specific properties. The performance approach establishes acceptable performance levels for the complete foam urethane and protective coating system and is based on the best information available. The format for performance levels consists of a stated requirement which is qualitative. This is a statement of how the system should perform under specific exposure conditions. Following this, a criterion states quantitatively the limiting value or values for performance in a specified test (example: the urethane foam shall attain a minimum of 95 percent adhesion to the substrate). Next, in order to evaluate the selected criterion, a test method is identified. Finally, a commentary is added, where appropriate, to place in perspective the relation of the test procedure and the criteria to performance of the roofing system in service.

¹Guidelines for Selection of and Use of Foam Polyurethane Roofing Systems, NBS Technical Note 778, in press.



Figure 1.

FFACTS

(FLAMMABLE FABRICS ACCIDENT)

"Brian, a 5-year-old pajama-clad male, was playing with matches. Although the first two matches ignited went out, the third continued burning and apparently fell into his lap, igniting the pajamas. The victim ran approximately 15-20 feet, where his mother, who had heard screams, met him. A blanket from the davenport was used to smother the flames. The victim suffered burns on 50 to 60 percent of his body and underwent seven skin grafts. Although neither parent smokes, leftover matches from a party held several weeks earlier were in an ash tray on the buffet. The parents were not concerned over the presence of matches since

the victim had never played with matches before his accident."

The case presented above, together with over 2,000 other case histories, are the foundation of the Bureau's Flammable Fabrics Accident Case and Testing System (FFACTS), a unique computerized inventory of fabric fire accidents. FFACTS collects case histories like this, quantifies them by translating words into numbers, tests fabric remnants to verify reports, and uses the resulting data to identify fabric flammability hazards. FFACTS is an important part of the Bureau's expanding National Fire Data System.

This case history is the result of

personal interviews with Brian and his family by a field investigator of the Bureau of Product Safety, FDA. The investigator may have to work his way through shock to obtain an accurate account of the incident for FFACTS. To alleviate this problem, one investigator says, "I always try to point out that the interview may help others avoid experiencing a fire." After listening to an unstructured account of what happened, the investigator uses a FFACTS questionnaire to piece together a concise yet comprehensive narrative about the incident. The case history, together with samples of the fabric involved, are sent to NBS for possible entry into FFACTS.

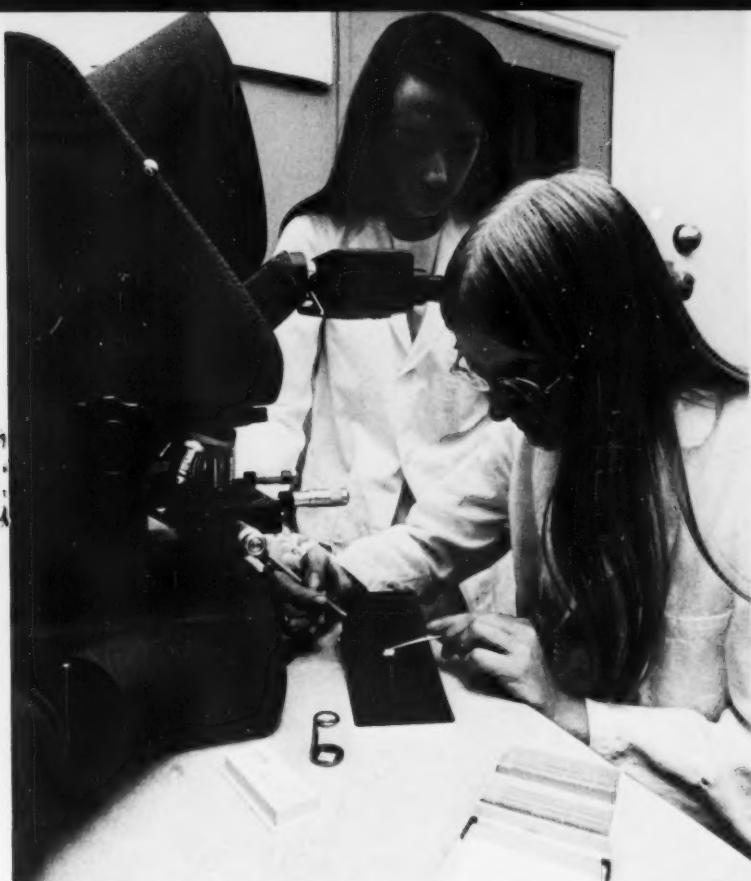


Figure 3.



Figure 2.



Figure 4.

NT CASE AND TESTING SYSTEMS)

The first step at NBS is to log in the case, label the fabric, and record such preliminary data as the area of the burn (Figure 1). "Opening the box gives me a feeling of sadness" said Mrs. Marjorie Hastedt, "especially when it contains a small garment, such as Brian's." Then too, the samples usually reek of smoke, are liable to break apart when handled, and often are wet from the water used to extinguish the fire.

Brian's case is then reviewed for possible entry into FFACTS (Figure 2). The case history must identify the fabric item involved in the fire and adequately explain how the ignition source contacted that item.

"About one case in five fails to meet FFACTS acceptance criteria," says Mr. Warren Hayes. "For instance, I once rejected a fabric fire case involving a dress thrown across a bed because the way it burned would not tell us anything about the way it would burn in normal use."

After the case was accepted, Mrs. Elaine Tyrrell (standing) and Miss Marilyn Baker (at microscope) prepare fabric specimens from Brian's pajamas for detailed examination (Figure 3). They identify the fiber by chemical and microscope tests, analyze the weave to determine fabric construction, measure the fabric weight, and conduct flammability tests. Their results

enable FFACTS to correlate fabric properties with the fabrics' role in the fire.

After screening, testing, and review, Brian's case and laboratory test results are coded for computer input by Miss Veronica Davis, a co-op student (Figure 4, left). Each case can have as many as 203 data elements, if all information is available. FFACTS tries to incorporate all relevant details of a fabric fire accident, including: victim's activity before the accident, ignition source, fabric characteristics, and extent of injuries. After coding, the case is edited to check the judgment used in "reading between
turn page



Figure 5.

FFACTS continued

the lines" of the case histories. The case is then keypunched by Mrs. Sadie Berry (Figure 4, right) and entered in the FFACTS computer base.

Mr. Peter Sun "questions" the computer for detailed information on sleepwear cases (Figure 5). The computer's answers often reveal fire accident patterns. Patterns ap-

pear in FFACTS data which involve such factors as age, activity, and ignition source and portray representative accident types. Analysis of accident patterns serves to identify prime causes and set priorities for action.

The curve in Figure 6 is a hazard analysis picture of accidental sleepwear fires according to age. It shows that young children and the elderly are most prone to suffer from flammable sleepwear. Mr. Henry Tovey, Chief of the Hazard Analysis Section, explains how this type of information is a primary consideration in determining flammability standard priorities.

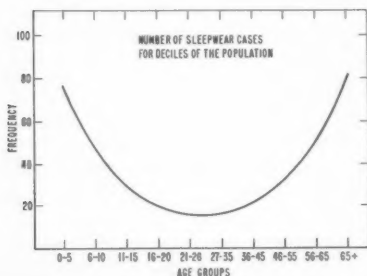
"A flammability standard covering all sleepwear is not yet practical since the supply of flame retardant fabric is limited and because some popular fabrics (e.g., polyester blends) cannot be made flame retardant. These data served as a basis

for the standard for children's sleepwear in sizes 0 through 6X aimed at protecting preschool children."

Brian's case highlights the hazard of children playing with matches, as well as the hazard of flammable sleepwear, according to Mr. Tovey. A survey of FFACTS data showed matches to be a major accidental ignition source in children's fire accidents, and has led to a government-industry effort to develop child-proof matches.

A Special Achievement Award in recognition of superior accomplishment for developing, implementing, and operating FFACTS in its early stages was presented to Mr. Richard Katz, Dr. Majorie Sandholzer, Miss Marilyn Baker, Mr. Allan Vickers, Mrs. Elaine Tyrrell, Mr. Robert Frye, and Mr. Jim Upberman (Computer Services Division).

Figure 6.



A NEW THEORY OF TOOTH DECAY

A new theory of tooth decay that could lead to new methods for prevention has been developed by Drs. Walter Brown and Prafull Patel, American Dental Association research associates in the Bureau's Dental Research Section. Their research was sponsored by NIH's National Institute of Dental Research. In a different approach to the problem, they theorize that the tooth surface acts as a permselective membrane—allowing calcium ions to leave the tooth and hydrogen ions to enter. This exchange increases the acidity within the tooth, causing more tooth mineral to dissolve and accelerating the diffusion of calcium ions.

Typically, the early stages of tooth decay involve substantial subsurface demineralization. The outer enamel layer, usually about 10 to 100 μm thick, exhibits hardly any loss of mineral. But beneath this is a partially demineralized region from which about half of the mineral has been dissolved. Separating the demineralized zone and the deeper, unaffected enamel is a relatively narrow region, the "reaction zone," where the degree of demineralization changes from about 50 percent to zero and which is the principal site of dissolution during active decay.

The theory advanced by Brown and Patel is aimed at explaining this subsurface demineralization. Essentially they say that the organic acids, principally lactic, produced by bacteria in the plaque are the primary cause of the demineralization. These acids diffuse into the tooth, causing some of the mineral to dissolve. This dissolution produces an elevated concentration

of calcium and phosphate ions within the tooth, causing these ions to diffuse out more rapidly than before the acid attack. If the plaque and the outer surface of the tooth act as a permselective membrane, restricting the flow of phosphate ions, then when the calcium ions move out they are replaced by hydrogen ions. Thus the acidity within the tooth is increased and the cycle continues.

Because of the difficulty of studying the caries process in an actual tooth, Brown and Patel studied saturated solutions of synthetic apatite. In their model system the caries lesion and the saliva are represented by compartments in a diffusion cell, and the outer layer of the tooth and the plaque are

represented by a cation exchange membrane. The laboratory results show that the concentrations of calcium, phosphate, and hydrogen ions within the tooth compartment are elevated by the diffusion process when the membrane restricts the flow of phosphate ions.

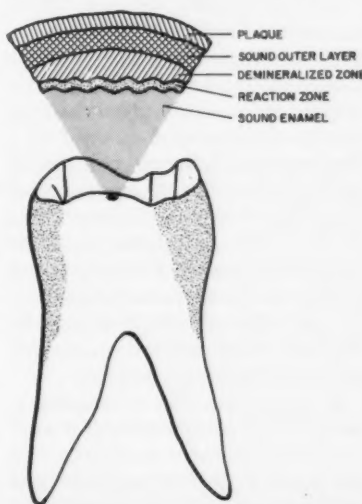
For example, in one experiment in which the tooth compartment contained hydroxyapatite dissolved in 0.001 M acetic acid and the saliva compartment contained 0.001 M acetic acid, the pH in the tooth compartment changed from 5.77 to 2.60 while that in the other compartment changed from 3.86 to 4.02.

These results cannot be translated directly to what may happen *in vivo*. However, Brown and Patel feel that it is particularly significant that the final pH in the tooth compartment, 2.60, was much lower than that in the saliva compartment, 4.02. It should also be recognized that an immense variety of conditions are found on tooth surfaces, and the probability is high that in some of these lactic acid-producing bacteria will be present at the same time as conditions that facilitate transport of calcium and hydrogen ions. Among such conditions are strong negative charges on the surfaces of enamel crystallites in the intact layer and in the plaque covering the tooth, and, possibly, electrical currents and voltages that would facilitate transport of calcium ions over phosphate ions.

If this theory proves to be correct, it will simplify the search for new decay preventives. Dr. Brown thinks that positively charged substances could be made that would keep the calcium in the tooth but

continued on page 126

The major features of tooth decay explained by Brown and Patel's new theory are shown in the expanded view of a caries lesion.



MATRIX ISOLATION STUDIES OF REACTIVE SPECIES



Dr. Jacox is shown here with part of the setup used in her matrix isolation studies.

Dr. Marilyn E. Jacox, a physical chemist in the Photochemistry Section of IMR, was one of six outstanding women to receive the 1973 Federal Woman's Award at a banquet on March 6, 1973. Through her research, Dr. Jacox has won international recognition as a specialist in infrared spectroscopy. She and her coworker, Dr. Dolphus Milligan, acting chief of the Photochemistry Section, have pioneered in the development of a technique for trapping and studying free radicals. Development of this matrix isolation technique has made it possible to characterize species that react so rapidly that they cannot be observed under normal laboratory conditions.

Born in Utica, N.Y., Dr. Jacox earned an A.B. in chemistry at Syracuse University's Utica College and a Ph. D. in physical chemistry at Cornell University. After completing her doctorate, she served as a Postdoctoral Research Associate at the University of North Carolina from May 1956 until October 1958. In November of 1958, she joined the Mellon Institute in Pittsburgh as a Fellow in Fundamental Research. She left Mellon in 1962 to join the Bureau's staff and continue her work in infrared spectroscopy.

Dr. Jacox is author or coauthor of 64 technical publications that have made significant contributions to the science of free radicals and molecular ions. Her previous honors

include the Outstanding Alumnus Award from Utica College (1963), the Washington Academy of Sciences Achievement Award in Physical Sciences (1969), and the Department of Commerce Gold Medal for Exceptional Service (1970).

Q. Congratulations on receiving the Federal Woman's Award for your outstanding work in infrared spectroscopy and free radical chemistry. Could you tell us what you look for when you study these very reactive species?

A. I'd like to say that all of this work has been a collaborative effort with Dr. Dolphus Milligan.

Basically, we take fingerprints of

molecules, usually molecules with five atoms or fewer, both organic and inorganic. In practice these fingerprints are primarily those given by the infrared spectrum of the molecule. In the infrared region of the spectrum there is an absorption pattern characteristic of different types of vibration of the atoms in the molecule. This pattern is strongly dependent on the masses of the individual atoms and readily measurable shifts occur in individual absorptions when heavy isotopic atoms are introduced into the molecule. This has been an extremely important factor in the analysis of our data.

To a lesser, but very significant extent, we also deal with the ultraviolet spectrum of the molecule. In this region of the spectrum, electronic transitions of the molecule occur, providing a different type of information. Mass effects are not detectable, the major exception being deuterium substitution for ordinary hydrogen.

Q. How do you trap free radicals and other reactive species so that they can be characterized?

A. In all of these experiments we have used the matrix isolation technique. In using this technique, we suspend the starting molecule in a large excess of an inert diluent, commonly argon or nitrogen, although it may be some other substance such as neon, carbon monoxide, carbon dioxide, or the heavier rare gases.

These materials have several essential properties; most of them are transparent over a very wide spectral region, and they can be frozen so that they're extremely rigid at temperatures below about 20 kelvin.

We freeze the sample containing the starting molecule of interest in an excess of diluent onto the cold cryostat window. Then, in many of our experiments, we subject the sample to ultraviolet or vacuum ultraviolet radiation, which induces

decomposition of the starting molecule, after which we determine the absorption spectrum of the trapped radicals.

Fragments are, of course, produced by photodecomposition. In one type of system each of the fragments contains two or more atoms. For example, a number of molecules of formula XN_3 decompose with elimination of molecular nitrogen. It happens that for many of these molecules the activation energy for recombination of NX with N_2 is high and at these low temperatures such a reaction is pretty effectively inhibited. Therefore, we are able to observe the absorption spectrum of the NX fragment directly, with a molecule of nitrogen trapped in an adjacent site in the argon lattice.

Q. Is everything in the system immobile at the temperatures you use?

A. Molecules cannot diffuse—not even diatomic molecules—at these low temperatures. However, atoms can diffuse to at least a limited extent. Now, if an atom is produced on photodecomposition of the molecule, it may migrate from the site of its photoproduction and leave an unstable reactive molecular fragment trapped at the site originally occupied by the stable molecule.

A diffusing atom can be exploited because of its potential of reacting with still another substance present in small concentration in the matrix. A number of the free radicals that we've seen are produced by such atom-molecule reactions. For example, we can introduce a photolytic source of hydrogen atoms in a matrix in which a small concentration of oxygen is present and observe appreciable concentrations of the free radical HO_2 in the infrared. This was the first triatomic free radical to be stabilized in an inert matrix environment; Dr. Milligan and I did this work back at the Mellon Institute about 11 years ago, a short time before we came to NBS.

Q. How many free radicals and molecular ions have you characterized thus far?

A. We've used the technique to obtain spectroscopic data for 60 or 70 small free radicals. Many of these are very essential reaction intermediates which, because they are molecular fragments, are chemically extremely reactive and not observable in conventional experimental systems because their steady state concentrations in a chemical process are below the limits of detection. We have also observed about 20 small molecular ions isolated in an argon matrix. This is a major but not complete focus of our current efforts.

I should mention a point regarding the characteristics of the spectrum. At these very low temperatures, for all but the simplest hydride molecules, rotational structures are completely quenched and we get a single sharp peak corresponding to a vibrational absorption in the matrix. This is very handy for isotopic substitution studies because we can measure quite accurately shifts in the vibration when heavy isotopes are substituted in the molecule. This has been crucial to identification of many of these free radicals and molecular ions.

Q. How do you analyze your data?

A. We use very sophisticated computer programs to obtain force constants, which tell us how strong the various chemical bonds in the molecule are in a rather semiquantitative way. This is especially important for free radicals and very reactive molecules because their reactivity is a result of some anomalies in their chemical bonding compared to stable molecules.

The information we get is also helpful in deducing the structures of these molecules. The number of vibrational absorptions in certain regions is the key to the structure for many molecules, and shifts on heavier isotopic substitution are ex-

tremely valuable in telling the number of atoms of certain types in the molecule and whether they move appreciably in any given vibration of the molecule. In favorable circumstances, we can obtain the vibrational contribution to the thermodynamic properties of the molecule using relatively simple calculations.

This information serves as a testing ground for existing theory and provides experimental data useful for extending theory as well. Our work has also increased knowledge of planetary atmospheres, essential to space probes, and provided valuable information on the combustion processes of flames.

Q. Can you pinpoint the major accomplishments of your studies?

A. One of our first major breakthroughs was the development of vacuum ultraviolet photolysis lamps with design and output suitable for coupling to matrix isolation experiments. This greatly extended the range of experiments that we could do and it's been exploited to a very considerable extent.

Another breakthrough involved our studies of cyanogen azide, NCN_3 , that we discovered decomposed first under rather gentle photolysis conditions to produce the expected products—molecular nitrogen plus the NCN species, which has a somewhat anomalous vibrational spectrum. Along the way we observed the known electronic transition for NCN and a new electronic transition. On more strenuous photolysis NCN photodecomposes, and the surprise is that it provides a source of carbon atoms. Both ordinary carbon-12 atoms and, because it's easy to introduce carbon-13 into the starting molecule, carbon-13 atoms are readily produced. We have been able to study the reaction of these carbon atoms with a number of other simple molecules present in matrix systems.

Photolytic sources of fluorine atoms have also been studied to a quite considerable extent and we have a body of literature in which products of these simple fluorine atom reactions are discussed.

Q. Is there one particular achievement that you would consider most outstanding?

A. The breakthrough in discovering that we could isolate molecular ions in a matrix was a singularly important one. Now it's true that a number of molecular ions are very familiar—inorganic ions, anions such as NO_2^- , NO_3^- , are commonly observed in crystals and in polar solutions. However, there was no guarantee at the start of this work that these would have the same structure or spectral properties if they were in a nonionic environment.

The first molecular ion that we identified was C_2^- , which we came upon quite accidentally in studies of the vacuum ultraviolet photolysis of acetylene in an argon or neon matrix. There were several anomalies in earlier studies in which the band system was identified as being due to the Swan system of C_2 .

Herzberg and Lagerqvist—Herzberg will be recognized as the recipient of the Nobel prize in chemistry 1 year ago—were working with flash discharges through gaseous methane and they discovered a new band system, which they demonstrated was due to a molecule of formula C_2 . But they were not able to find a pair of low-lying electronic levels for neutral C_2 to which it was possible to assign this new gas phase transition. They suggested that it might be due to a negatively charged molecule, namely C_2^- . They wrote urging us to do further experiments to see whether we might confirm this because this would be the first negatively charged molecule for which a gas phase spectrum had ever been detected.

Well, after some time and some

thought such an experiment was devised. When we introduced a small concentration of cesium atoms, which provided a very convenient source of photoelectrons, into the system, we observed a dramatic increase in the concentration of this molecule, providing very strong support for the assignment of the transition to C_2^- instead of to the Swan bands of C_2 . Since then there have been matrix isolation and gas phase studies in other laboratories that also support the reassignment.

In more general terms our major contribution was to find the conditions suitable for stabilizing such reactive species in inert matrices. We are beginning to lay down ground rules for the production of molecular ions, and I think this is going to be equally significant in the long run.

Q. You mentioned earlier that you had done some work on combustion intermediates. Could you tell us a little about the specific systems that were involved in your work?

A. We discovered that the C-H bond of HCO , a combustion intermediate, is anomalously weak. I shouldn't say we alone discovered this, it's been recognized in electron spin resonance studies of HCO as well. But it is important to determine the position of CH stretching absorption in the infrared spectrum on this molecule. We were able to obtain all three of the vibrational fundamentals of HCO and of DCO some years ago. For many years people have studied a very complicated group of perhaps 100 emission bands in the visible ultraviolet region of the spectrum, which appeared on observation of a wide variety of hydrocarbons—these were called the hydrocarbon flame bands. It was believed, but not definitively established, that they were contributed by HCO .

Well, we had the ground state vibrational constants for HCO , and we found that we could produce an

ultraviolet absorption system by preparing HCO in a matrix at low temperatures. We could then get the upper state vibrational constants of this transition. The origin of the transition corresponded quite closely to that which had been determined for the hydrocarbon flame bands. With this number of constants then, we were able to demonstrate that this absorption system was indeed due to HCO because we'd established the conditions for making it in excellent yield in the infrared studies, and we were able to provide a complete vibrational assignment for the hydrocarbon flame bands as a result of determining these individual vibrational constants in both the upper and the lower states. Since then we've analyzed the data in somewhat greater detail, and we hope soon to write a brief note in which we present evidence for the occurrence of still another electronic transition of HCO in the general region of the hydrocarbon flame bands.

Q. How does your work contribute to understanding upper atmosphere or space phenomena?

A. Both O_3^- and O_4^- are very important chemical intermediates in processes characteristic of the earth's ionosphere. We have obtained vibrational data for these species and have observed an electronic transition for O_3^- as well, although this had previously been



Dr. Jacox and Dr. Milligan, Acting Chief of the Photochemistry Section, examine the infrared spectrum of a free radical. Both scientists have received awards for their contributions to free radical chemistry: Dr. Jacox the Federal Woman's Award, and Dr. Milligan the first Professor Arturo Miolati Prize for outstanding scientific achievement in 1966.

observed in crystals. This I think is important in the space effort.

Another thing that is important in the space effort is studies of the molecule CO_3 , first produced by Warren Thompson and two of his graduate students at Case Western Reserve. We were able to confirm these experimental studies and extend them somewhat. Our work confirmed their assignment of the spectrum to CO_3 rather than to a molecule that still might have contained hydrogen. Also, we were able to do an elaborate vibrational analysis of the data and to determine a reasonably good structure for CO_3 . I think this is important both from the

standpoint of the theory and the standpoint of CO_3 itself, which may be an intermediate in various planetary atmospheric reactions, since CO_2 at a rather low temperature predominates in the Martian atmospheres and at a rather high temperature in the atmosphere of Venus. So CO_3 has to be reckoned with as a possible intermediate in processes there. Photochemists have done a lot of work on the possible role of CO_3 in these atmospheres. There's question about how well it holds together at temperatures characteristic of Mars and Venus. This is a question we'd like to do more work on.

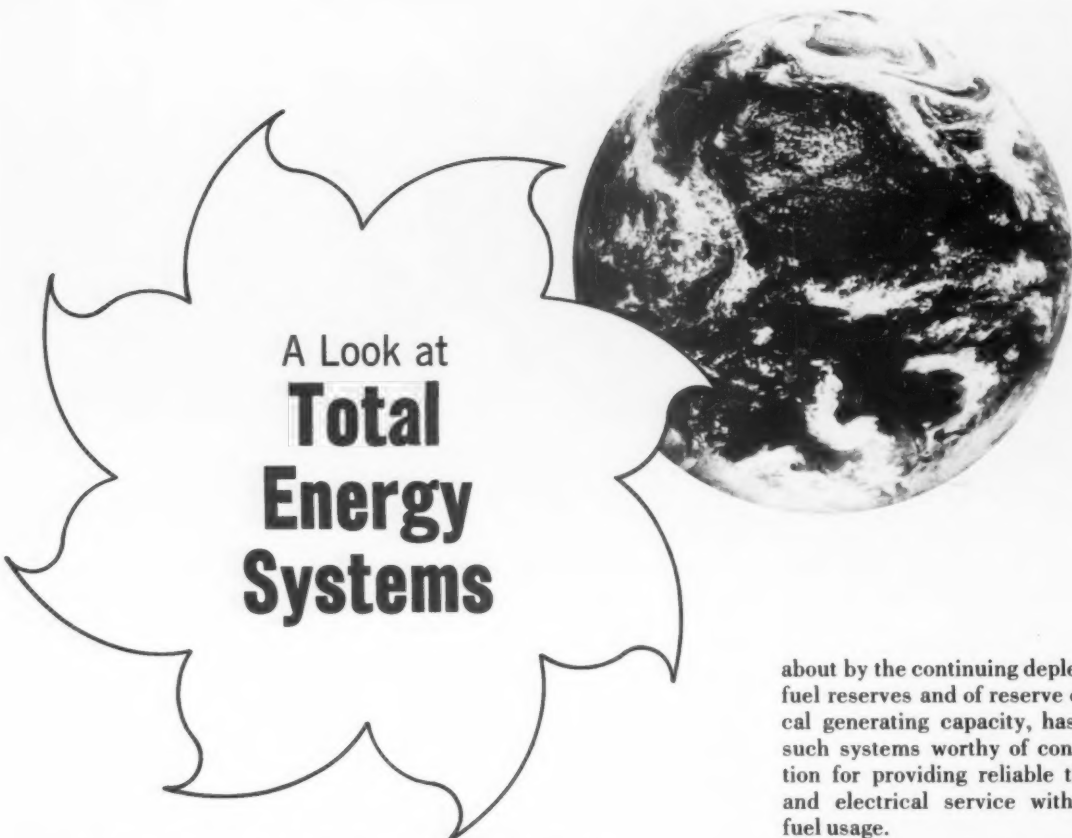


Research Associate Develops Fire Test

Dr. Richard W. Roberts, right, makes his first presentation of a Research Associate certificate of appreciation since assuming directorship of the National Bureau of Standards. The recipient is L. Gene Hartzell, who received the commendation upon completion of his 1 year Research Associate Program under the sponsorship of Arm-

strong Cork Company on the subject of flooring fire test methods.

During his year at NBS Hartzell developed and validated a small scale test method for flooring materials, which correlates with fire exposure in full-scale situations. Use of the test will reduce significantly the cost of evaluating the flammability of materials.



A Look at **Total Energy Systems**

Properly designed total energy systems could achieve energy savings of 28 to 40 percent if applied to medium-size housing developments in six selected areas of the United States, according to an NBS study.

A forecast of new housing patterns by Paul R. Achenbach and John B. Coble of the Center for Building Technology indicates that total energy systems might potentially serve as much as 20 percent of the new housing market.¹ Application of total energy systems on this scale could save enough energy to supply all of the electrical and thermal needs of an additional 200,000 dwelling units, Achenbach and Coble report.

In a total energy system—which

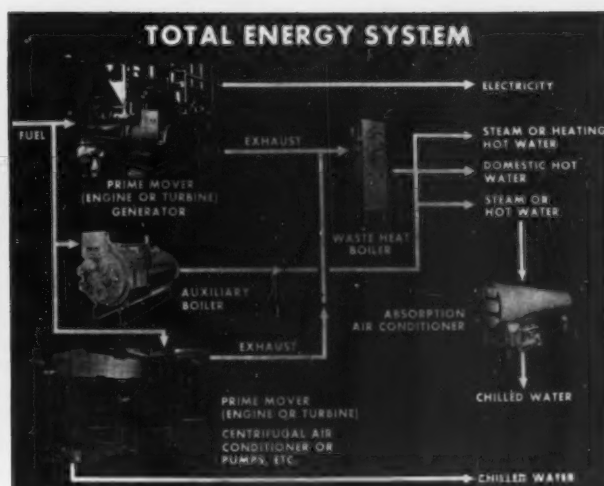
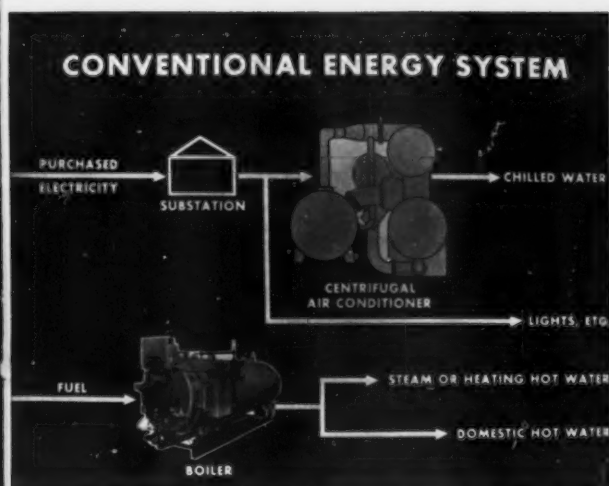
generally serves a single large building or a building complex within a single site—fuel-burning engine generators provide electricity and heat for hot water and space heating or cooling. Though they are not considered practical for single dwelling units, the advantage of total energy systems over conventional central generating stations is that about half the energy wasted in conventional power plants can be reclaimed.

The U.S. energy crisis, brought

about by the continuing depletion of fuel reserves and of reserve electrical generating capacity, has made such systems worthy of consideration for providing reliable thermal and electrical service with lower fuel usage.

The total energy concept is now new. Since 1958 about 600 systems ranging in size from 0.2 to 20 megawatts have been installed in the United States. More recently, however, the number of new total energy plants installed annually has decreased sharply. A significant number of smaller total energy systems has been discontinued because of high maintenance costs and poor reliability. Although 550 systems are currently in use, very little published data is available regarding their effectiveness for residential applications.

In 1970 the U.S. Department of Housing and Urban Development asked the Center for Building Technology to examine the feasibility of applying experimentally total energy systems to six prototype **BREAKTHROUGH** housing sites



These figures illustrate the principal components of a conventional energy system and a total energy system.

and to develop reliable data on these systems as primary utility options.

The study analyzed the magnitude and diversity of the electrical and thermal loads, the various combinations of mechanical equipment available, the dwelling unit density and arrangement, energy costs, owning and operating costs, housing designs, community planning, and compatibility of a total energy system with the development schedules at the several sites.

Preliminary findings led to the recommendation to go ahead with a full-scale field study of a total energy plant, for which the Jersey City BREAKTHROUGH site was selected. The Jersey City total energy plant will serve four medium- to high-rise apartment buildings, two schools, about 45,000 square feet of light commercial space, and a swimming pool. Overall site dimensions are about 1,400 by 700 feet.

The total energy plant is built around five 600-kilowatt diesel generators which produce all the electricity for the site. The heat from the cooling water and exhaust

gases of the diesel generators provides heating, air conditioning (using absorption chillers) and domestic hot water for the site buildings. The electricity, chilled water and hot water generated in the Central Equipment Building (CEB) are distributed in underground conduits. The Central Equipment Building also houses a pneumatic trash collection system which is the subject of a field study on this site.

The energy field study is being directed by Paul R. Achenbach, Chief of the Building Environment Division, and consists of six activities:

- a. *An energy use study.* Continuous measurement, for a year or more, of the fuel used, electrical energy and heat generated, excess heat discarded, and the use of electrical energy by all major segments of the load. These data will be used to calculate overall plant thermal efficiency.
- b. *Performance of major plant components.*
- c. *Electrical service stability.*
- d. *Service reliability.*

e. *Environmental conditions.* Collection of information on noise, combustion effluents, air pollution, cooling tower effluents, thermal conditions, and other environmental data for comparison with the requirements of NBS performance specifications.

f. *Owning and operating costs.* Construction of the total energy plant at Jersey City began early in the spring of 1972 and plant operation is expected within the year.

It is anticipated that the results obtained from this particular site can be reliably extrapolated to larger housing developments elsewhere, to some variations in combinations of building types on other proposed sites, and to installations where different fuel and labor costs are in effect. The results are expected to constitute a good technical base for guiding the wider application of total energy plants.

¹ Achenbach, P. R., and Cable, J. B., Site Analysis for the Application of Total Energy Systems to Housing Developments, Proceedings of the 7th Intersociety Energy Conversion Engineering Conference, San Diego, 1972.



NEWS

After this issue, the NSRDS News will no longer appear in the Technical News Bulletin but will be distributed as a separate newsletter. Those presently on the NSRDS News mailing list will automatically receive the newsletter. Interested Bulletin readers may arrange to receive the NSRDS News by writing to:

Office of Standard Reference Data
National Bureau of Standards
Washington, D.C. 20234.

SUBROUTINE FOR CALCULATION OF CODEN CHECK CHARACTERS

CODEN for journal titles are abbreviations, such as JNBAA for *Journal of Research of the National Bureau of Standards, Physics and Chemistry*, that provide a completely defined, short, frequently mnemonic identifier for a serial publication. This system is maintained by the American Society for Testing and Materials (ASTM) and is used both by information systems and some scientific journals. The recently published NBS Technical Note 738, *Subroutine for the Calculation of CODEN Check Characters* by David Garvin,¹ Director of the NBS Chemical Kinetics Information Center (SD Catalog No. C13.46:738, 25 cents), describes a FORTRAN subroutine that computes the check character for an ASTM CODEN for journal titles.

This routine, written for input in Hollerith characters, is adaptable to other coding schemes. A listing of the routine is provided in NBS Technical Note 738.

RADIATION CHEMISTRY DATA CENTER CUMULATIVE INDEX

The latest *Index and Cumulative List of Papers on Radiation Chemistry* covering the period July through December 1972 has been issued by the University of Notre Dame Radiation Chemistry Data Center. The more than 18,000 references were obtained by scanning 40 appropriate current journals, chemical abstracts, and nuclear abstracts. References are grouped into the following categories: radiation chemistry, polymers, biological systems, hot-atom chemistry, ESR, luminescence, photochemistry, theoretical studies, and miscellaneous.

The *Cumulative Index* may be ordered from the National Technical Information Service, Springfield, Va. 22151, for the price of \$6. It bears the number COM-73-10281.

ARGON, 1970: INTERNATIONAL THERMODYNAMIC TABLES OF THE FLUID STATE

The Thermodynamic Tables Project was inaugurated by the Commission on Thermodynamics and Thermochemistry of the Division of Physical Chemistry of the International Union of Pure and Applied Chemistry, with the object of compiling internationally agreed values

of the equilibrium thermodynamic properties of liquids and gases of interest to both scientists and technologists. The range to be covered for each fluid is that for which there exist reliable experimental data, and the agreed values will be issued as tables which users may use as a basis for producing equations suited to their own special requirements. The present publication contains the following data and tables relating to argon: physical constants and fixed points, vapor pressure equations, PVT surface equations, derived properties, the IUPAC Tables, saturation properties, single-phase properties, and tolerance diagrams. In the United States and Canada, the book may be ordered from Crane, Russak & Co., Inc., 52 Vanderbilt Avenue, New York, N.Y. 10017, for \$12.50. Overseas the book is available from the publisher, Butterworth & Co. Ltd., 88 Kingsway, London WC2B 6AB, for £5 plus 30p for postage.

EVALUATED KINETIC DATA COMPILATIONS

Two compilations of evaluated kinetic data have recently been published as a result of work carried out on projects at the Department of Chemistry, Birmingham University, supported by the Office for Scientific and Technical Information of the United Kingdom.

The first volume, *Evaluated Kinetic Data and Gas Phase Addition Reactions: Reactions of Atoms and Radicals with Alkenes, Alkynes*

and Aromatic Compounds by J. A. Kerr and M. J. Parsonage, London: Butterworths, 1972, 384 pages, £12 (\$30), brings together quantitative kinetic data on gas-phase addition reactions. It is a compilation of critically evaluated rate data for the reactions of atoms and radicals with unsaturated molecules, covering the literature up to the end of 1970. A 16-page introduction deals with theory and assumptions used in compiling the selected data, such as the orientation of addition to asymmetrical olefins, A-factors for addition reactions, reactivity and molecular structure of substrate molecules, and the nature of the transition state in addition reactions. The major part of the book presents absolute rate constants and Arrhenius parameters in the form of data sheets, one or more for each pair of reactants. There is also a section dealing with the relative rate data. An author, as well as a subject index makes it easy for the reader to ascertain quickly if rate data are available for a particular addition reaction.

The second volume, *Second Supplementary Tables of Bimolecular Gas Reactions* by J. A. Kerr and E. Ratajczak, supplements *Tables of Bimolecular Gas Reactions* by A. F. Trotman-Dickenson and G. Milne,¹ NSRDS-NBS-9 (SD Catalog No. C13.48:9, \$2), 1967, and *Supplementary Tables of Bimolecular Gas Reactions* by E. Ratajczak and A. F. Trotman-Dickenson, UWIST, Cardiff, 1969. It comprises sets of tables of kinetic data (rate constants, activation energies, and A-factors) for bimolecular gas-phase reactions. Most of the results refer to transfer processes involving atoms and radicals reacting with molecules, but the latest supplement includes tables on atom/radical combinations and addition reactions. The work covers the literature issued during the period January 1969 to December 1971. Copies

of the *Second Supplementary Tables* are available from Dr. J. A. Kerr, Department of Chemistry, Haworth Building, The University, Birmingham B15 2TT, for £1 (\$2.50) post free.

COMPILATION FROM CERN AVAILABLE

Compilation of Cross Sections— $I-\pi^-$ and π^+ Induced Reactions (CERN/HERA 72-1) by E. Bracci, J. P. Droulez, E. Flaminio, J. D. Hansen, and D. R. O. Morrison is a compilation of cross sections of reactions produced by negative and positive pions on targets of protons, neutrons, and deuterons. This is an updated version of CERN/HERA 70-5 and 70-7 and contains 40 percent more data values than the earlier publications. Graphs of the variation of cross section with incident laboratory momentum are plotted. Values of the rate of decrease of cross section with incident momentum are given. The compilation is available in the Western Hemisphere and Far East from Lawrence Berkeley Laboratory, Berkeley, Calif. 94720; users elsewhere should order from CERN, Geneva, Switzerland.

TRANSLATION OF COMPENDIUM OF CONSTITUTIONAL TERNARY DIAGRAM

A Compendium of Constitutional Ternary Diagrams of Metallic Systems by W. Guertler, M. Guertler, and E. Anastasiadis has been translated by J. Schmorak for the Israel Program for Scientific Translations, Jerusalem 1969. This work, first published in Germany in 1959, contains phase diagrams for 243 metallic systems including all binary and ternary alloys of manganese, iron, cobalt, nickel, copper, palladium, silver, platinum, and gold. In those cases where the ternary diagrams were not complete or available in the open literature, they have been constructed from the most reliable binary diagrams

available. The *Compendium* may be ordered from the National Technical Information Service, Springfield, Va. 22151, as TT 69-55069 for \$10.

NBS STANDARDS INFORMATION SERVICES (SIS)

The NBS Engineering and Product Standards Division maintains a service for providing up-to-date information on standards and standardization activities in the United States. The SIS has a reference collection of engineering and related standards which includes over 20,000 standards, specifications, test methods, codes, and recommended practices issued by more than 380 U.S. technical societies, professional organizations, and trade associations. The collection also contains: specifications of state purchasing offices; standards and specifications of U.S. Government agencies; standards and specifications of the major foreign and international standardizing bodies; and over 600 technical reference books, including directories, encyclopedias, guides, and manuals, and more than 70 periodicals and newsletters.

The SIS also functions as a referral activity by directing inquirers to appropriate standards-issuing organizations. By means of a computer-produced Key-Word-In-Context (KWIC) Index, the SIS is able to provide answers to questions on standards.

To obtain SIS information, write to:

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TOOTH DECAY *continued*

Dr. Patel prepares a diffusion cell. The crystal-containing solution on the left is separated from the acid on the right by a cation exchange membrane.

allow phosphate to leach out. The loss of phosphate would make the tooth less acid and encourage the formation of apatite crystals.

The American Dental Association has sponsored a substantial Research Associate effort at NBS for nearly 40 years. This program has encouraged unusually close rapport among this physical science laboratory, dental manufacturers, and practicing dentists. A number of major developments now in everyday use—the high-speed drill, the panoramic x-ray machine, and a variety of improved filling materials—have resulted from this program.



Proposed Standard for Dense Numeric Representations

Proposed standard formats for packing numeric data on a magnetic tape, disk pack, or cassette for computer processing and information interchange have been drafted by the Bureau. The packing of numeric data allows more data to be recorded on a medium and doubles the transmission speed for numeric data.

NBS is now accepting comments on the draft standard—Federal Information Processing Standard Publication (FIPS PUB) on Representations of Numerical Data in Dense Forms for Information Exchange. Copies of the proposed standard may be obtained from, and

comments should be submitted to:
Office of Information
Processing Standards
Room B-264, Technology
Building
Washington, D.C. 20234
Telephone: (301) 921-3545

The Federal Government has developed this standard for dense forms to increase the efficiency of Federal computer use and information interchange. The computer industry has implemented various methods for representing dense numeric forms. There has been little interest by the industry in the development of such a standard because of the investment in current systems.

This proposed standard is intended to augment ASCII (the American Standard Code for Information Interchange) and provides for representation of numeric data in a more effective form. ASCII is now widely used in telecommunications, but its growth as a computer processing code has been less

rapid, due in part to the lack of a standard for associated compact data forms.

Dense data forms have been employed in third and fourth generation computer systems where character framing is in 8-bit aggregations. One of the dense forms in the proposal, called "packed decimal numeric" data, provides a 4-bit representation for each decimal digit, algebraic sign, and separator. Thus, two characters can be packed into the 9-bit octet (byte) normally allocated to one character of a larger set, such as ASCII. Another dense form is "binary" and the third dense form is "floating point binary."

Comments on the proposal are welcomed. Responses will be most helpful to NBS in making decisions on future actions on this standard. Early responses will also be considered by FIPS Task Group 12 that is conducting a study on the significance and impact of ASCII as a Federal standard.

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